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Note

Exponential Difference Operator Approximation for the Sixth Order Onsager Equation

Introduction

The construction of difference approximations for complicated operators by building them from successive applications of standard difference operators can be algebraically tedious and therefore prone to the introduction of errors. Standard methods for generating difference approximations based on Taylor series also frequently yield poor acccuracy when the operators involve variable coefficients or when variable mesh zoning is used. The finite element method is a more systematic method of approximation well suited to variable meshes and complicated boundary conditions, but again the computation of coefficients can be algebraically very tedious if the partial differential operators become at all complicated.

An alternative is to use exponential difference operator approximation formulas [1–4]. These are easy to program, but do not yet seem to be widely applied. In part this may be because the advantages they have in ease of application and accuracy are not so apparent in the low order derivative uniform mesh problems which have often been used to demonstrate them. This note gives an application of these methods to a complicated approximation problem involving sixth order derivatives on a nonuniform mesh.

The equation discussed describes the flow in a countercurrent gas centrifuge and is of practical interest in the field of uranium enrichment [5–8]. It is derived from the Navier–Stokes equations after linearization and the dropping of a number of terms.

A one-dimensional form of the sixth order Onsager equation is

$$L^6\psi = (e^x(e^x\psi_x)_{xx})_{xxx} = f(x), \tag{1}$$

with boundary conditions at $x = 0$,

$$\psi = 0, \tag{2}$$

$$\psi_x = 0, \tag{3}$$

$$(e^x(e^x\psi_x)_{xx})_x = \gamma, \tag{4}$$

at $x = x_\infty$,

$$\psi = 0, \tag{5}$$

$$(e^x\psi_x)_x = 0, \tag{6}$$

$$(e^x(e^x\psi_x)_{xx})_{xx} = 0. \tag{7}$$

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As one can appreciate after a little reflection and experimentation, the construction of a finite difference or finite element approximation to this equation and boundary conditions is not a trivial task, yet the method to be described is very easy to program and debug. This is an important point as in many applications the time and costs required to set up and program a solution method are many times the actual cost of computing solutions.

Method and Test Problems

The key to the method is to note that over a small interval the function f can be replaced by a constant. In practice f could represent a complicated dependence on x in one dimension or it could represent an operator with respect to another coordinate in the case of two dimensions. Whichever the case, one replaces f by a constant C_{1k}. This constant is then regarded as an unknown in developing the difference approximation for L^6 at the kth mesh point. The example equation

$$L^6\psi = C_{1k} \tag{8}$$

can be solved exactly to obtain an analytical approximation for ψ in the neighborhood of the kth mesh point. This solution introduces six additional unknown constants C_i. Most nth order differential operator equations of this form can be integrated exactly resulting in a closed form solution with $n+1$ unknown constants C_i, but even cases which can only be solved by series methods can be included with little additional computation. The analytical solution to $L^6\psi = C_1$ obtained by successive integrations is

$$\begin{aligned}\psi = &- C_1(\tfrac{1}{12}x^3 + \tfrac{5}{8}x^2 + \tfrac{17}{8}x + \tfrac{49}{16})\, e^{-2x} \\ &- C_2(\tfrac{1}{4}x^2 + \tfrac{5}{4}x + \tfrac{17}{8})\, e^{-2x} - C_3(\tfrac{1}{2}x + \tfrac{5}{4})\, e^{-2x} \\ &- \tfrac{1}{2}C_4 e^{-2x} - C_5(x+1)\, e^{-x} - C_6 e^{-x} + C_7.\end{aligned} \tag{9}$$

To construct the difference approximation for the example equation at an interior mesh point k, one requires that the analytical solution with the seven unknowns including C_1 equal the finite difference solution at mesh points $k-3$, $k-2$, $k-1$, k, $k+1$, $k+2$, and $k+3$. Thus one has a set of seven linear equations in the seven unknowns C_i which must be solved at each interior mesh point k;

$$\begin{aligned}&-(\tfrac{1}{12}x_{k+i}^3 + \tfrac{5}{8}x_{k+i}^2 + \tfrac{17}{8}x_{k+i} + \tfrac{49}{16})\, e^{-2x_{k+i}}C_{1k}, \\ &-(\tfrac{1}{4}x_{k+i}^2 + \tfrac{5}{4}x_{k+i} + \tfrac{17}{8})\, e^{-2x_{k+i}}C_{2k}, \\ &-(\tfrac{1}{2}x_{k+i} + \tfrac{5}{4})\, e^{-2x_{k+i}}C_{3k} - \tfrac{1}{2}e^{-2x_{k+i}}C_{4k}, \\ &-(x_{k+i}+1)\, e^{-x_{k+i}}C_{5k} - e^{-x_{k+i}}C_{6k} + C_{7k} = \psi_{k+i},\end{aligned} \tag{10}$$

where $i = -3, -2, -1, 0, 1, 2, 3$.

Since $C_{1k} \equiv L^6\psi_k$ one obtains an approximation for $L^6\psi_k$ in terms of the value ψ_k and its six neighboring mesh values from the top row of the inverse of the 7×7 matrix of coefficients multiplying the column vector (C_{1k}, C_{2k}, C_{3k}, C_{4k}, C_{5k}, C_{6k}, C_{7k}). Thus if i goes from -3 to $+3$, then Eq. (10) can be written

$$A_{i+4,j}(x_k)\, C_{j,k} = \psi_{k+i} \tag{11}$$

which can be solved for the C_{jk} yielding

$$C_{jk} = A^{-1}_{ji+4}\psi_{k+i}. \tag{12}$$

The approximation for $L^6\psi$ obtained from Eq. (8) is then

$$(e^x(e^x\psi_x)_{xx})_{xxx}|_{x=x_k} \equiv C_{1k} = \sum_{i=-3}^{3} B_{k,i+4}\psi_{k+i}, \tag{13}$$

where $B_{ki} = A^{-1}_{1,i}(x_k)$.

These steps have been written out in detail to show the nature of the approximation, and to state it in a form in which boundary conditions are easily treated. Normally one would be able to write the seven independent functions appearing in Eq. (10) by inspection. In the present case these functions are

$$\psi_n(x) = 1, \quad e^{-x}, \quad xe^{-x}, \quad e^{-2x}, \quad xe^{-2x}, \quad x^2e^{-2x}, \quad x^3e^{-2x}. \tag{14}$$

The coefficients B_{ki} in the difference approximation at the kth interior mesh point must satisfy

$$L^6\psi_n(x_k) = \sum_{i=1}^{7} B_{ki}\psi_n(x_{k+i-4}) \tag{15}$$

which yields a system of seven equations, one for each ψ_n, in the seven unknown values of B_i at the kth mesh point.

Boundary conditions are easily included by replacing the equations that would otherwise involve virtual boundary mesh points with the equations for the appropriate derivatives at the boundary. In the example problem at the boundaries $x_1 = 0$, $x_{k\,\max} = x_\infty$ the function values are zero, and need not be computed. At the mesh point x_2 the interior equations (10) for $i = -2$ and -3 are replaced by using Eq. (9) in the analytical boundary conditions (3) and (4), yielding

$$4C_{12} + 3C_{22} + 2C_{32} + C_{42} + C_{62} = 0, \tag{16}$$

$$C_{32} = \gamma. \tag{17}$$

At the mesh point x_3 the interior equation (10) for $i = -3$ is replaced by Eq. (16).

Similarly at the mesh point $x_{k\,\max-1}$ the interior equations (10) for $i=2$ and 3 are replaced using Eq. (9) in the analytical boundary conditions (6) and (7), yielding

$$\begin{aligned} &-\tfrac{1}{6}(x^3_{k\,\max}+3x^2_{k\,\max}+6x_{k\,\max}+6)\,e^{-x_{k\,\max}}C_1,\\ &\quad -\tfrac{1}{2}(x^2_{k\,\max}+2x_{k\,\max}+2)\,e^{-x_{k\,\max}}C_2,\\ &\quad -(x_{k\,\max}+1)\,e^{-x_{k\,\max}}C_3-e^{-x_{k\,\max}}C_4+C_5=0, \end{aligned} \tag{18}$$

and

$$C_1x_{k\,\max}+C_2=0. \tag{19}$$

Finally at mesh point $x_{k\,\max-2}$ the interior equation (10) for $i=3$ is replaced by Eq. (18).

Since boundary condition (4) is inhomogeneous, in the present case the corresponding form of Eq. (13) for the mesh points at x_2 is

$$(e^x(e^x\psi_x)_{xx})_{xxx}|_{x=x_2}=\sum_{i=-1}^{3}B_{2,i+4}\psi_{2+i}-B_{2,1}\gamma. \tag{20}$$

Thus at the end points of the mesh the approximation for the differential operator involves a linear combination of the interior mesh values and the derivatives of ψ at the boundary. In the present example the remaining equations are:

at $x=x_3$,

$$(e^x(e^x\psi_x)_{xx})_{xxx}|_{x=x_3}=\sum_{i=-2}^{3}B_{3,i+4}\psi_{3+i}, \tag{21}$$

at $x=x_{k\,\max-2}$,

$$(e^x(e^x\psi_x)_{xx})_{xxx}|_{x=x_{k\,\max-2}}=\sum_{i=-3}^{2}B_{k\,\max-2,i+4}\psi_{k\,\max-2+i}, \tag{22}$$

at $x=x_{k\,\max-1}$

$$(e^x(e^x\psi_x)_{xx})_{xxx}|_{x=x_{k\,\max-1}}=\sum_{i=-3}^{1}B_{k\,\max-1,i+4}\psi_{k\,\max-1+i}. \tag{23}$$

One obtains a banded discrete set of equations approximating differential equation (1) and boundary conditions (2)–(7) by equating the expressions for the operator L^6, Eqs. (13), (20)–(23), to the corresponding mesh point values $f_k=f(x_k)$.

The mesh point values ψ_k obtained from the solution of this banded system of linear equations are exact for the case $f=$ constant and very good approximate solutions for general $f(x)$. The programming of the method is simple and aided by the circumstance that one can usually find an exact solution for the case $f=0$ with which to compare to check for coding errors. In the present example the solution to the homogeneous case $f=0$, $\gamma=1$ is

$$\psi(x) = -\tfrac{1}{2}(x+1)\,e^{-2x} + \tfrac{1}{2}e^{-x} \tag{24}$$

in the limit $x_\infty \to \infty$. The comparison between the solution by Eq. (24) and the discrete approximation for a variable mesh of 50 points is shown in Table I. This

TABLE I

K, *X*, Analytical Solution, Numerical Approximation

1	0.	0.	1.73372E-10
2	1.04000E-01	2.27436E-03	2.27429E-03
3	2.12160E-01	7.91131E-03	7.91106E-03
4	3.24646E-01	1.53838E-02	1.53833E-02
5	4.41632E-01	2.34853E-02	2.34844E-02
6	5.63298E-01	3.13045E-02	3.13034E-02
7	6.89829E-01	3.81959E-02	3.81945E-02
8	8.21423E-01	4.37449E-02	4.37432E-02
9	9.58280E-01	4.77326E-02	4.77308E-02
10	1.10061E+00	5.00988E-02	5.00968E-02
11	1.24864E+00	5.09062E-02	5.09041E-02
12	1.40258E+00	5.03062E-02	5.03041E-02
13	1.56268E+00	4.85089E-02	4.85068E-02
14	1.72919E+00	4.57556E-02	4.57535E-02
15	1.90236E+00	4.22969E-02	4.22949E-02
16	2.08245E+00	3.83750E-02	3.83731E-02
17	2.26975E+00	3.42106E-02	3.42088E-02
18	2.46454E+00	2.99942E-02	2.99926E-02
19	2.66712E+00	2.58816E-02	2.58802E-02
20	2.87781E+00	2.19924E-02	2.19912E-02
21	3.09692E+00	1.84112E-02	1.84101E-02
22	3.32480E+00	1.51906E-02	1.51896E-02
23	3.56179E+00	1.23559E-02	1.23550E-02
24	3.80826E+00	9.90993E-03	9.90922E-03
25	4.06459E+00	7.83846E-03	7.83786E-03
26	4.33117E+00	6.11496E-03	6.11445E-03
27	4.60842E+00	4.70517E-03	4.70473E-03
28	4.89676E+00	3.57083E-03	3.57046E-03
29	5.19663E+00	2.67267E-03	2.67236E-03
30	5.50849E+00	1.97267E-03	1.97240E-03
31	5.83283E+00	1.43556E-03	1.43532E-03
32	6.17015E+00	1.02979E-03	1.02958E-03
33	6.52095E+00	7.27982E-04	7.27795E-04
34	6.88579E+00	5.06984E-04	5.06813E-04
35	7.26522E+00	3.47701E-04	3.47542E-04
36	7.65983E+00	2.34731E-04	2.34581E-04
37	8.07022E+00	1.55913E-04	1.55769E-04
38	8.49703E+00	1.01839E-04	1.01700E-04
39	8.94091E+00	6.53754E-05	6.52396E-05
40	9.40255E+00	4.12212E-05	4.10876E-05
41	9.88265E+00	2.55121E-05	2.53800E-05
42	1.03820E+01	1.54878E-05	1.53566E-05
43	1.09012E+01	9.21567E-06	9.08519E-06
44.	1.14413E+01	5.37061E-06	5.24054E-06
45	1.20029E+01	3.06285E-06	2.93303E-06
46	1.25871E+01	1.70789E-06	1.57823E-06
47	1.31945E+01	9.30343E-07	8.00776E-07
48	1.38263E+01	4.94617E-07	3.65104E-07
49	1.44834E+01	2.56400E-07	1.26918E-07
50	1.51667E+01	1.29464E-07	0.

table demonstrates that there are no problems with round-off errors, matrix conditioning, or truncated boundary conditions. Equation (24) is slightly in error for the largest x values since the right-hand boundary is at 15.1667 rather than infinity.

In the general case one would be replacing f in Eq. (1) by some complex, perhaps nonlinear, function of ψ or by an operator on ψ in another dimension. The accuracy

TABLE II

K, X, Analytical Solution, Numerical Approximation

1	0.	0.	1.94224E-08
2	1.04000E-01	3.16853E-03	3.15905E-03
3	2.12160E-01	1.12591E-02	1.12254E-02
4	3.24646E-01	2.23599E-02	2.22931E-02
5	4.41632E-01	3.48524E-02	3.47485E-02
6	5.63298E-01	4.74167E-02	4.72755E-02
7	6.89829E-01	5.90281E-02	5.88525E-02
8	8.21423E-01	6.89438E-02	6.87392E-02
9	9.58280E-01	7.66815E-02	7.64543E-02
10	1.10061E+00	8.19908E-02	8.17483E-02
11	1.24864E+00	8.48194E-02	8.45691E-02
12	1.40258E+00	8.52768E-02	8.50256E-02
13	1.56268E+00	8.35951E-02	8.33493E-02
14	1.72919E+00	8.00924E-02	7.98571E-02
15	1.90236E+00	7.51364E-02	7.49159E-02
16	2.08245E+00	6.91137E-02	6.89109E-02
17	2.26975E+00	6.24029E-02	6.22196E-02
18	2.46454E+00	5.53537E-02	5.51906E-02
19	2.66712E+00	4.82715E-02	4.81285E-02
20	2.87781E+00	4.14084E-02	4.12846E-02
21	3.09692E+00	3.49584E-02	3.48528E-02
22	3.32480E+00	2.90579E-02	2.89691E-02
23	3.56179E+00	2.37890E-02	2.37154E-02
24	3.80826E+00	1.91872E-02	1.91272E-02
25	4.06459E+00	1.52499E-02	1.52017E-02
26	4.33117E+00	1.19459E-02	1.19077E-02
27	4.60842E+00	9.22376E-03	9.19405E-03
28	4.89676E+00	7.02044E-03	6.99761E-03
29	5.19663E+00	5.26729E-03	5.24999E-03
30	5.50849E+00	3.89540E-03	3.88247E-03
31	5.83283E+00	2.83930E-03	2.82977E-03
32	6.17015E+00	2.03935E-03	2.03241E-03
33	6.52095E+00	1.44311E-03	1.43811E-03
34	6.88579E+00	1.00580E-03	1.00223E-03
35	7.26522E+00	6.90217E-04	6.87677E-04
36	7.65983E+00	4.66172E-04	4.64370E-04
37	8.07022E+00	3.09744E-04	3.08459E-04
38	8.49703E+00	2.02367E-04	2.01437E-04
39	8.94091E+00	1.29932E-04	1.29243E-04
40	9.40255E+00	8.19365E-05	8.14063E-05
41	9.88265E+00	5.07154E-05	5.02893E-05
42	1.03820E+01	3.07898E-05	3.04301E-05
43	1.09012E+01	1.83215E-05	1.80035E-05
44	1.14413E+01	1.06775E-05	1.03851E-05
45	1.20029E+01	6.08944E-06	5.81241E-06
46	1.25871E+01	3.39561E-06	3.12763E-06
47	1.31945E+01	1.84970E-06	1.58693E-06
48	1.38263E+01	9.83399E-07	7.23542E-07
49	1.44834E+01	5.09776E-07	2.51519E-07
50	1.51667E+01	2.57402E-07	0.

of this method for such applications can be illustrated by comparing numerical and exact solutions for the case $f(x)=\delta(x_0-x)$, $\gamma=0$. Since the solution is the Green's function for the problem comparison with the exact solution shows the propagation of the errors introduced in the neighborhood of the δ function by the approximation. In contrast with the first example, the accuracy deteriorates as the number of mesh

TABLE III

K, *X*, Analytical Solution, Numerical Approximation

1	0.	0.	-1.08262E-08
2	1.00000E-01	2.92630E-03	2.92508E-03
3	2.00000E-01	1.01138E-02	1.01095E-02
4	3.00000E-01	1.96560E-02	1.96475E-02
5	4.00000E-01	3.01751E-02	3.01619E-02
6	5.00000E-01	4.07045E-02	4.06864E-02
7	6.00000E-01	5.05931E-02	5.05701E-02
8	7.00000E-01	5.94290E-02	5.94015E-02
9	8.00000E-01	6.69788E-02	6.69470E-02
10	9.00000E-01	7.31394E-02	7.31040E-02
11	1.00000E+00	7.79010E-02	7.78624E-02
12	1.20000E+00	8.34846E-02	8.34411E-02
13	1.40000E+00	8.45677E-02	8.45213E-02
14	1.60000E+00	8.22200E-02	8.21725E-02
15	1.80000E+00	7.74875E-02	7.74400E-02
16	2.00000E+00	7.12732E-02	7.12268E-02
17	2.20000E+00	6.42967E-02	6.42521E-02
18	2.40000E+00	5.70959E-02	5.70536E-02
19	2.60000E+00	5.00491E-02	5.00094E-02
20	2.80000E+00	4.34037E-02	4.33665E-02
21	3.00000E+00	3.73054E-02	3.72712E-02
22	3.20000E+00	3.18248E-02	3.17938E-02
23	3.40000E+00	2.69793E-02	2.69515E-02
24	3.60000E+00	2.27506E-02	2.27261E-02
25	3.80000E+00	1.90991E-02	1.90776E-02
26	4.00000E+00	1.59731E-02	1.59544E-02
27	4.20000E+00	1.33158E-02	1.32998E-02
28	4.40000E+00	1.10704E-02	1.10567E-02
29	4.60000E+00	9.18236E-03	9.17072E-03
30	4.80000E+00	7.60132E-03	7.59148E-03
31	5.00000E+00	6.28198E-03	6.27370E-03
32	5.20000E+00	5.18424E-03	5.17729E-03
33	5.40000E+00	4.27315E-03	4.26734E-03
34	5.60000E+00	3.51856E-03	3.51370E-03
35	5.80000E+00	2.89468E-03	2.89063E-03
36	6.00000E+00	2.37966E-03	2.37628E-03
37	6.20000E+00	1.95503E-03	1.95222E-03
38	6.40000E+00	1.60532E-03	1.60297E-03
39	6.60000E+00	1.31756E-03	1.31561E-03
40	6.80000E+00	1.08097E-03	1.07934E-03
41	7.00000E+00	8.86574E-04	8.85214E-04
42	8.00000E+00	3.27912E-04	3.27334E-04
43	9.00000E+00	1.20904E-04	1.20620E-04
44	1.00000E+01	4.45197E-05	4.43451E-05
45	1.10000E+01	1.63841E-05	1.62501E-05
46	1.20000E+01	6.02830E-06	5.90927E-06
47	1.30000E+01	2.21783E-06	2.10433E-06
48	1.40000E+01	8.15913E-07	7.04457E-07
49	1.50000E+01	3.00160E-07	1.89459E-07
50	1.60000E+01	1.10423E-07	0.

points is reduced since in this case the numerical solution is only an approximation. Table II shows the comparison for a 50-point mesh with $x_0 = 2.66712$. The agreement between the exact solution and the numerical approximation is excellent, even though the δ function is approximated by

$$\begin{aligned} f_k &= -2/(x_{k+1} - x_{k-1}), \qquad & x_k &= x_0, \\ &= 0, & x_k &\neq x_0. \end{aligned} \tag{25}$$

This discrete approximation method can also accommodate large discontinuous jumps in mesh spacing without loss of accuracy. Table III shows a similar 50-point case $f(x) = \delta(x_0 - x)$, $\gamma = 0$, $x_0 = 2.60000$, computed on a mesh which is uniform except for two places; at $x = 1.0$ the mesh size doubles from 0.1 to 0.2 and at $x = 7.0$ the mesh size increases 5× from 0.2 to 1.0. Again the agreement between the exact and discrete approximation solutions is excellent.

Table IV shows the previous case again but with half the number of mesh points. The accuracy of the discrete approximation is still good despite the extreme variation of the driving function and the crudeness of the mesh; however, the accuracy begins to deteriorate more noticibly when the number of mesh points is reduced further.

TABLE IV

K, *X*, Analytical Solution, Numerical Approximation

1	0.	0.	-1.31261E-10
2	2.00000E-01	1.01138E-02	1.00975E-02
3	4.00000E-01	3.01751E-02	3.01246E-02
4	6.00000E-01	5.05931E-02	5.05051E-02
5	8.00000E-01	6.69788E-02	6.68571E-02
6	1.00000E+00	7.79010E-02	7.77528E-02
7	1.40000E+00	8.45677E-02	8.43897E-02
8	1.80000E+00	7.74875E-02	7.73048E-02
9	2.20000E+00	6.42967E-02	6.41248E-02
10	2.60000E+00	5.00491E-02	4.98955E-02
11	3.00000E+00	3.73054E-02	3.71725E-02
12	3.40000E+00	2.69793E-02	2.68709E-02
13	3.80000E+00	1.90991E-02	1.90152E-02
14	4.20000E+00	1.33158E-02	1.32533E-02
15	4.60000E+00	9.18236E-03	9.13712E-03
16	5.00000E+00	6.28198E-03	6.24990E-03
17	5.40000E+00	4.27315E-03	4.25075E-03
18	5.80000E+00	2.89468E-03	2.87921E-03
19	6.20000E+00	1.95503E-03	1.94442E-03
20	6.60000E+00	1.31756E-03	1.31033E-03
21	7.00000E+00	8.86574E-04	8.81657E-04
22	9.00000E+00	1.20904E-04	1.20189E-04
23	1.10000E+01	1.63841E-05	1.62519E-05
24	1.30000E+01	2.21783E-06	2.16499E-06
25	1.50000E+01	3.00160E-07	2.58081E-07
26	1.70000E+01	4.06225E-08	0.

Conclusions

The exponential operator method of approximating derivatives and partial derivatives is easy to program and provides good accuracy for higher order complex differential operators on variable meshes. Boundary conditions are included naturally such that the approximations at points adjacent to the boundaries are stated in terms of derivatives at the boundary. Thus the desired boundary conditions can be specified exactly without the use of virtual mesh points or other approximations. Because the mesh point coefficients are derived from an analytic solution to a local approximation of the differential or partial differential equation the method can tolerate large jumps in mesh spacing without loss of accuracy.

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